FIGURE 1A

A

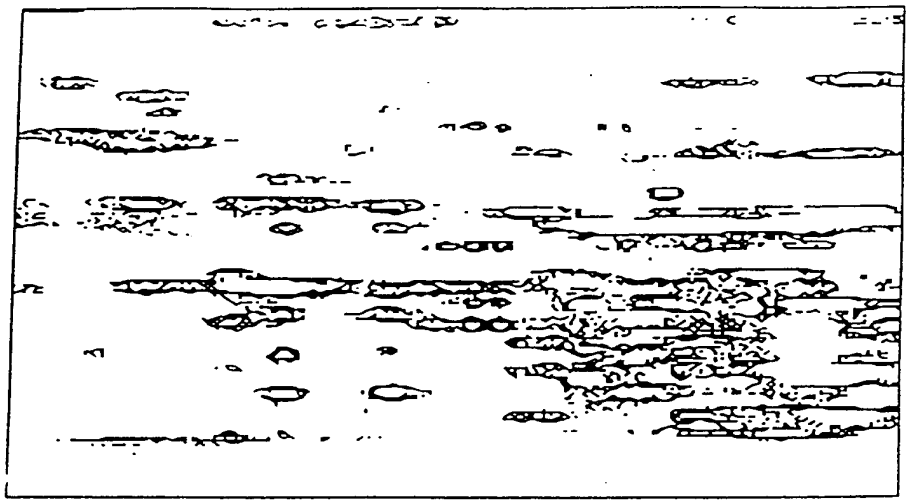


FIGURE 1B

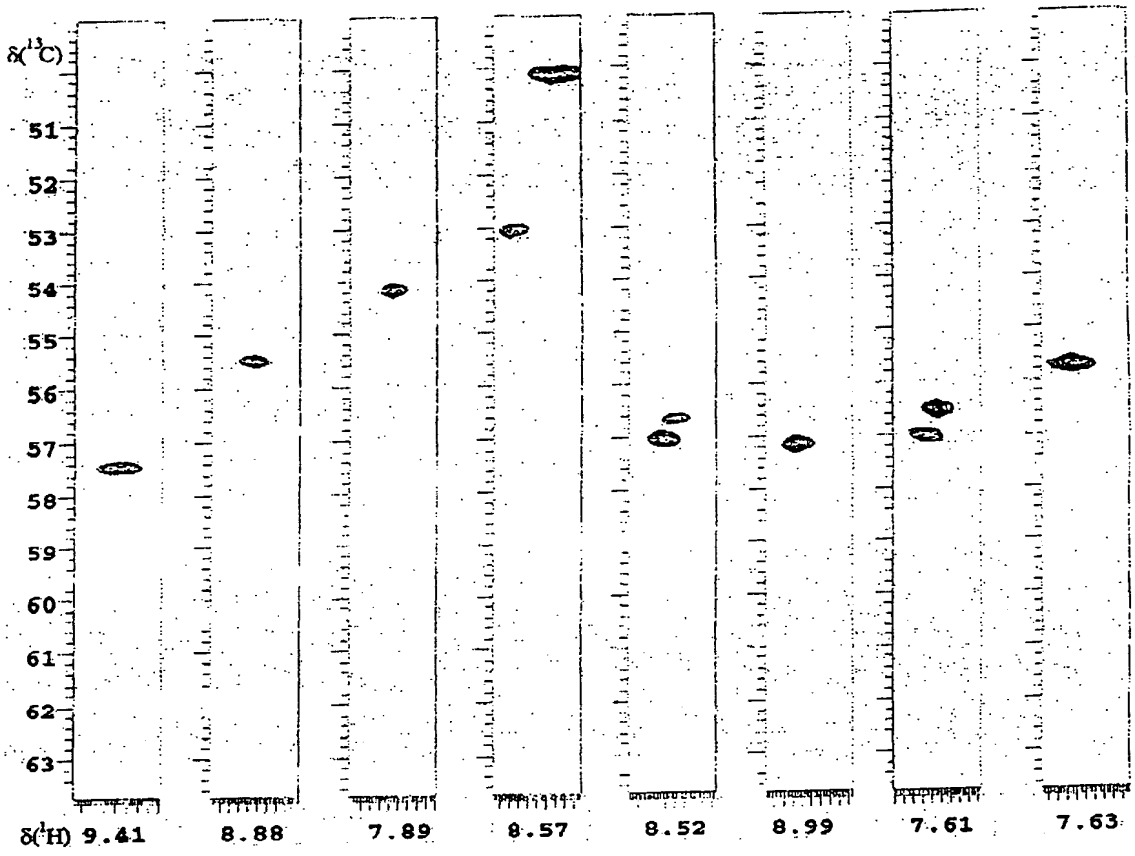
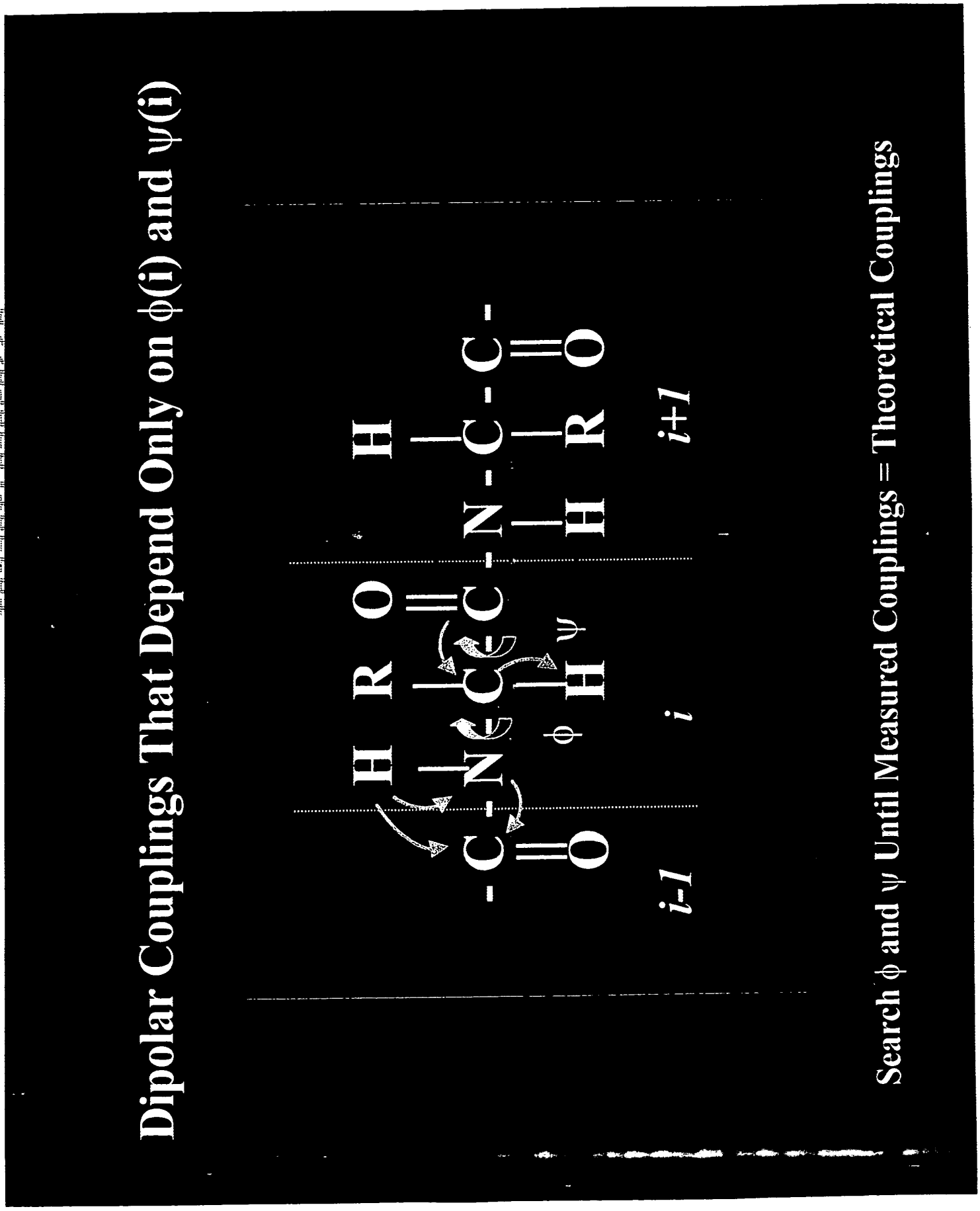


FIGURE 2


Dipolar Couplings That Depend Only on φ(i) and ψ(i)
H R O H
-C-N-C-C-N-C-C-
O H ψ
φ
i-1 i i+1
Search φ and ψ Until Measured Couplings = Theoretical Couplings

Packing Secondary Structural Elements

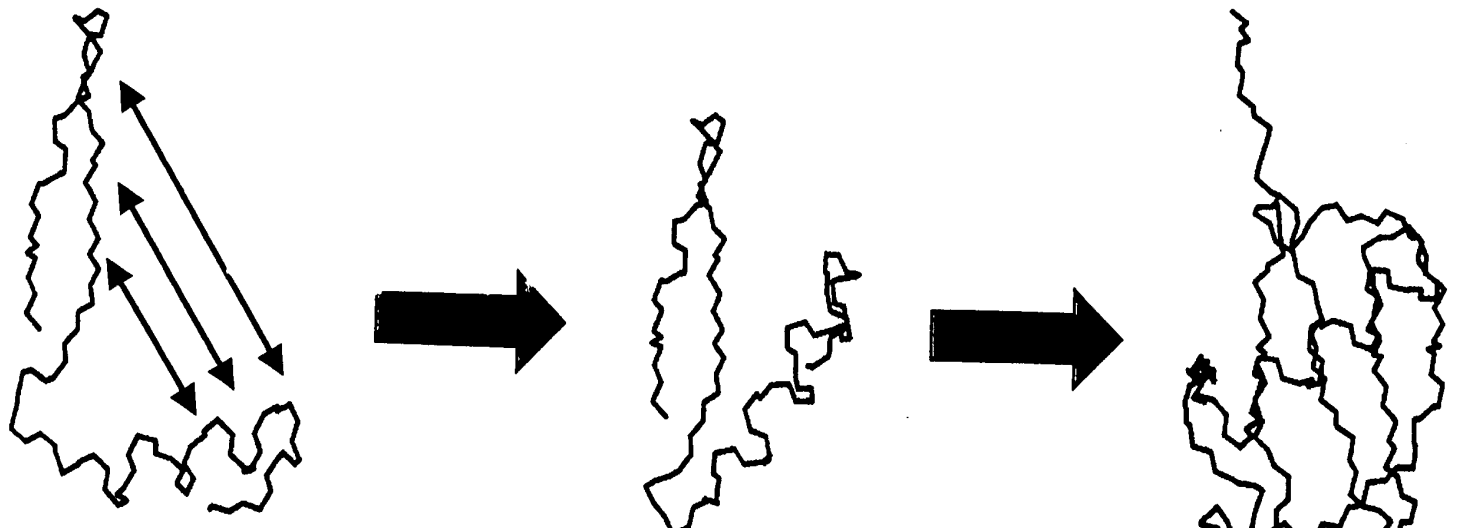
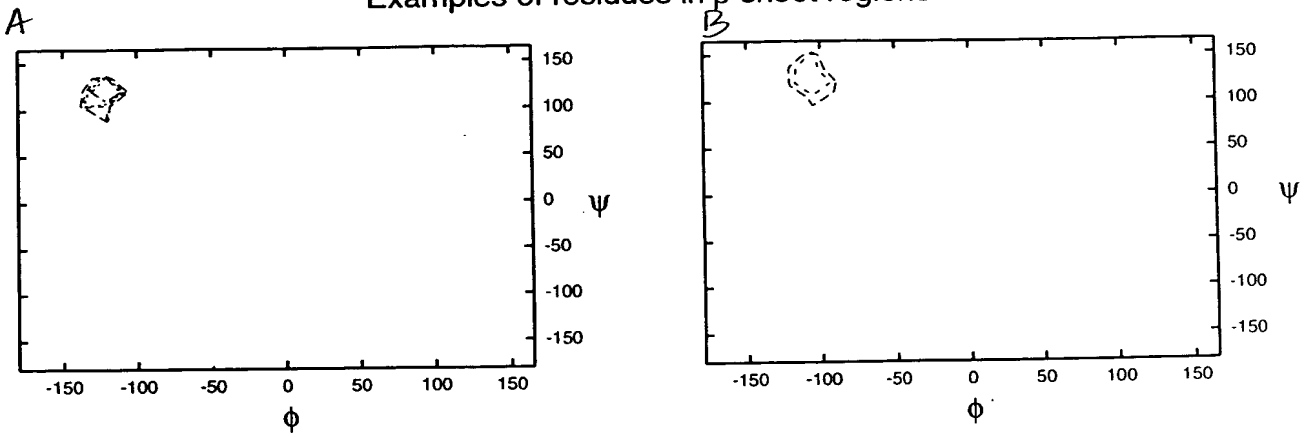
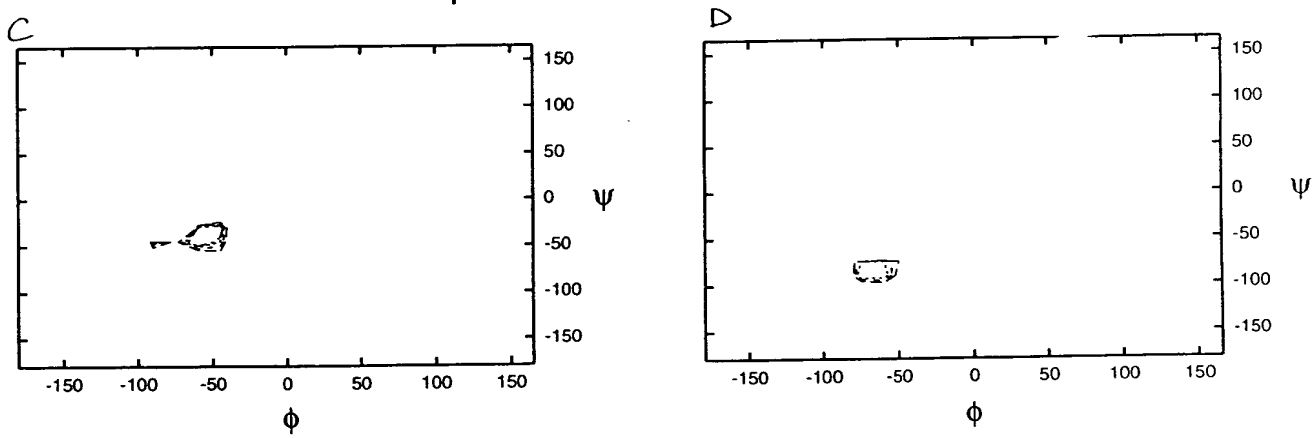


FIGURE 4

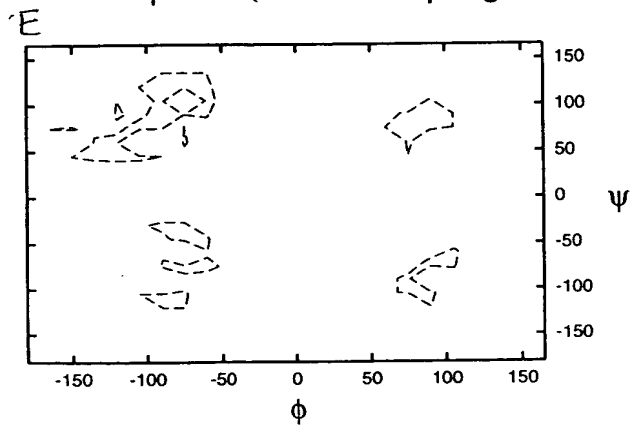
Examples of residues in β-sheet regions



Examples of residues in α-helix regions



Example of residue in loop region



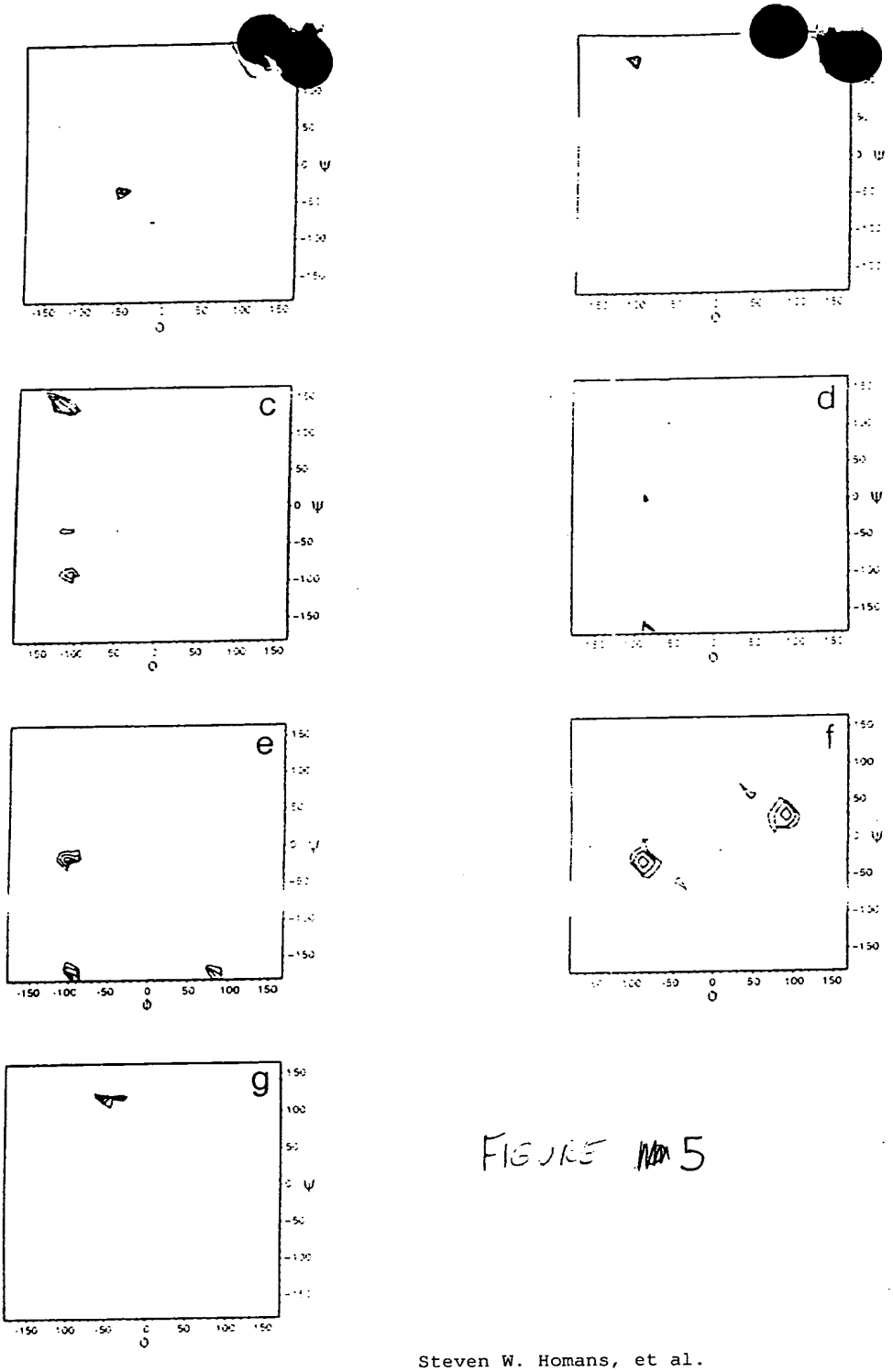


FIGURE No 5

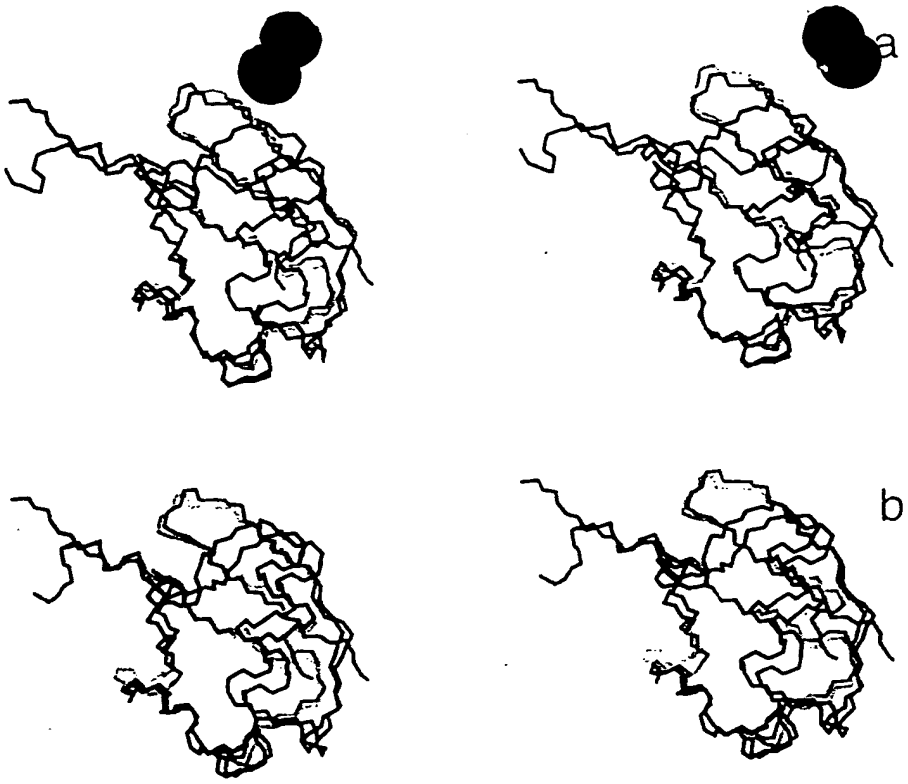


FIGURE 6

FIGURE 7

Generate Linear amino-acid chain

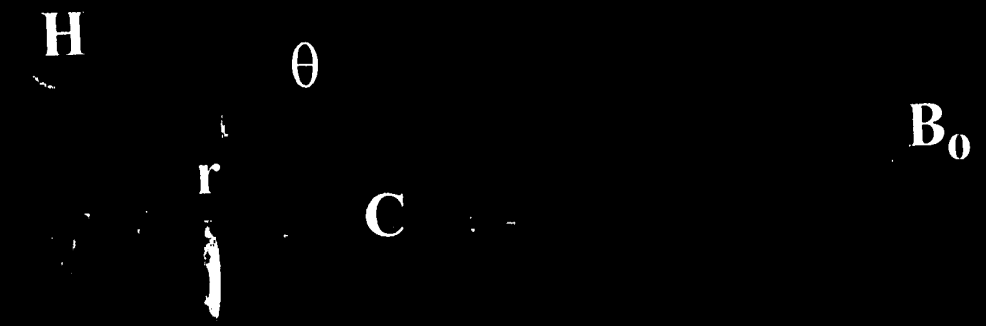
Calculate ϕ, ψ angles for each peptide pair using experimental residual dipolar couplings

Fold Linear sequence with dihedral angle and backbone NOE restraints

Refine structure using NOE and dipolar coupling restraints

FIGURE 8

Dipolar Couplings - Powerful Structural Constraints



$$D \alpha (3 \cos^2\theta - 1) / r^3$$

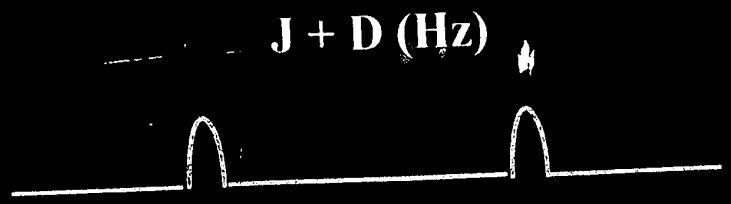
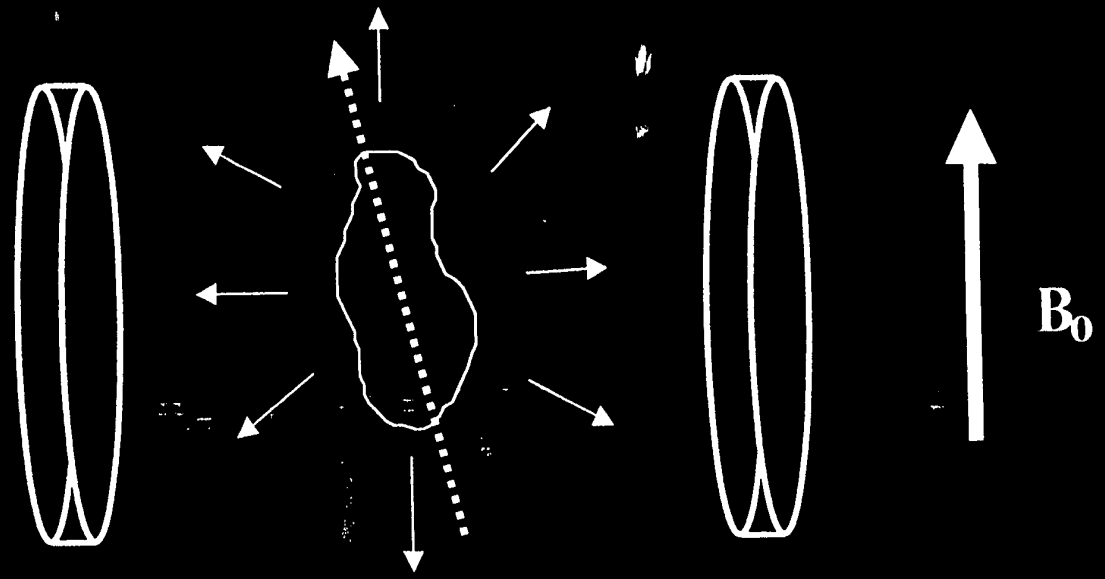


FIGURE 9

Measurement of Dipolar Couplings Requires a Weakly Aligned Molecule



Phospholipid Bicelles

J (Hz)

22° C: Isotropic (no alignment)

J + D (Hz)

35° C: LC Phase (alignment)

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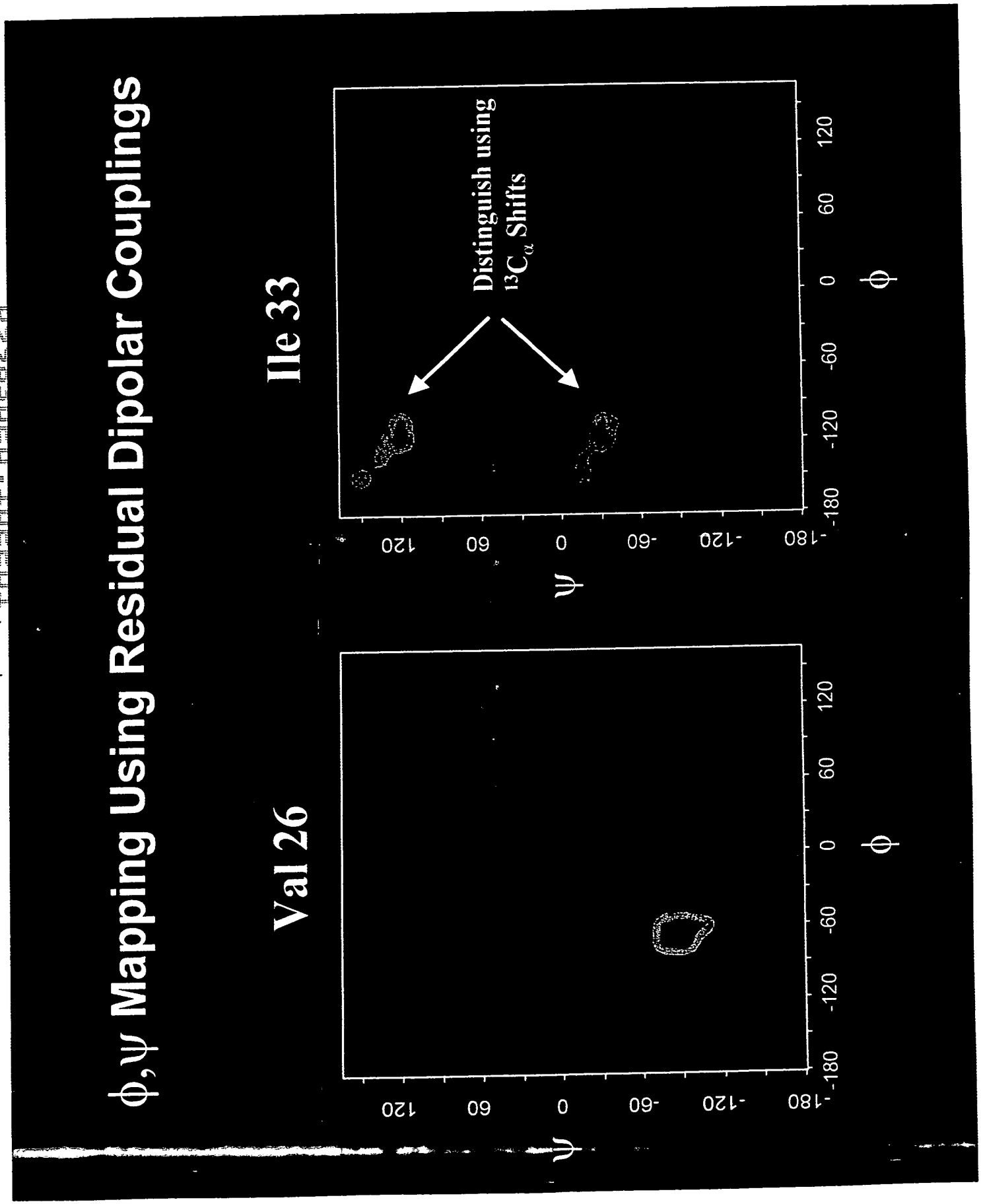
FIGURE 10


φ,ψ Mapping Using Residual Dipolar Couplings
Ile 33
Distinguish using
$^{13}C_\alpha$ Shifts
Val 26
ψ
φ
120
60
0
-60
-120
-180

16

FIGURE 11

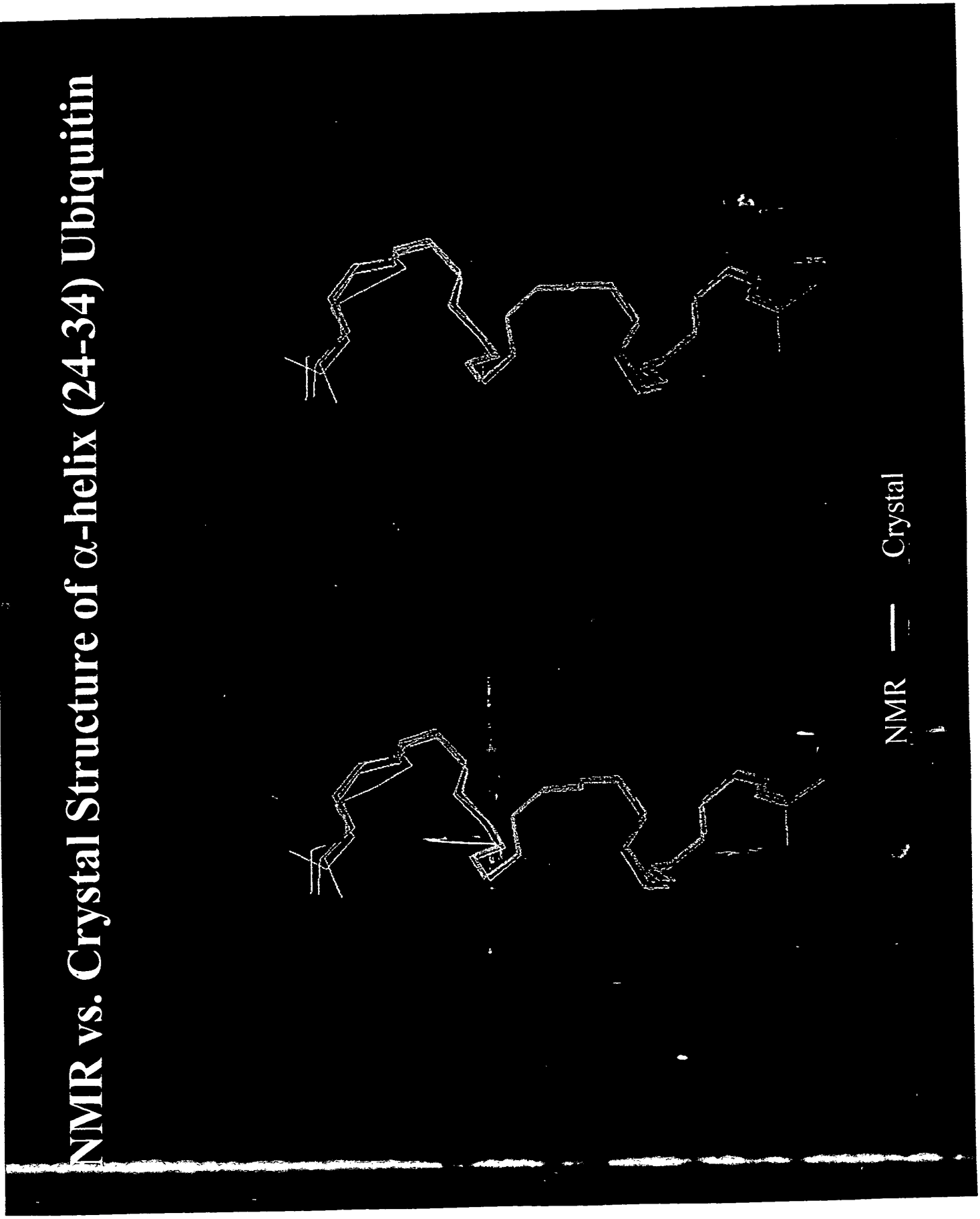
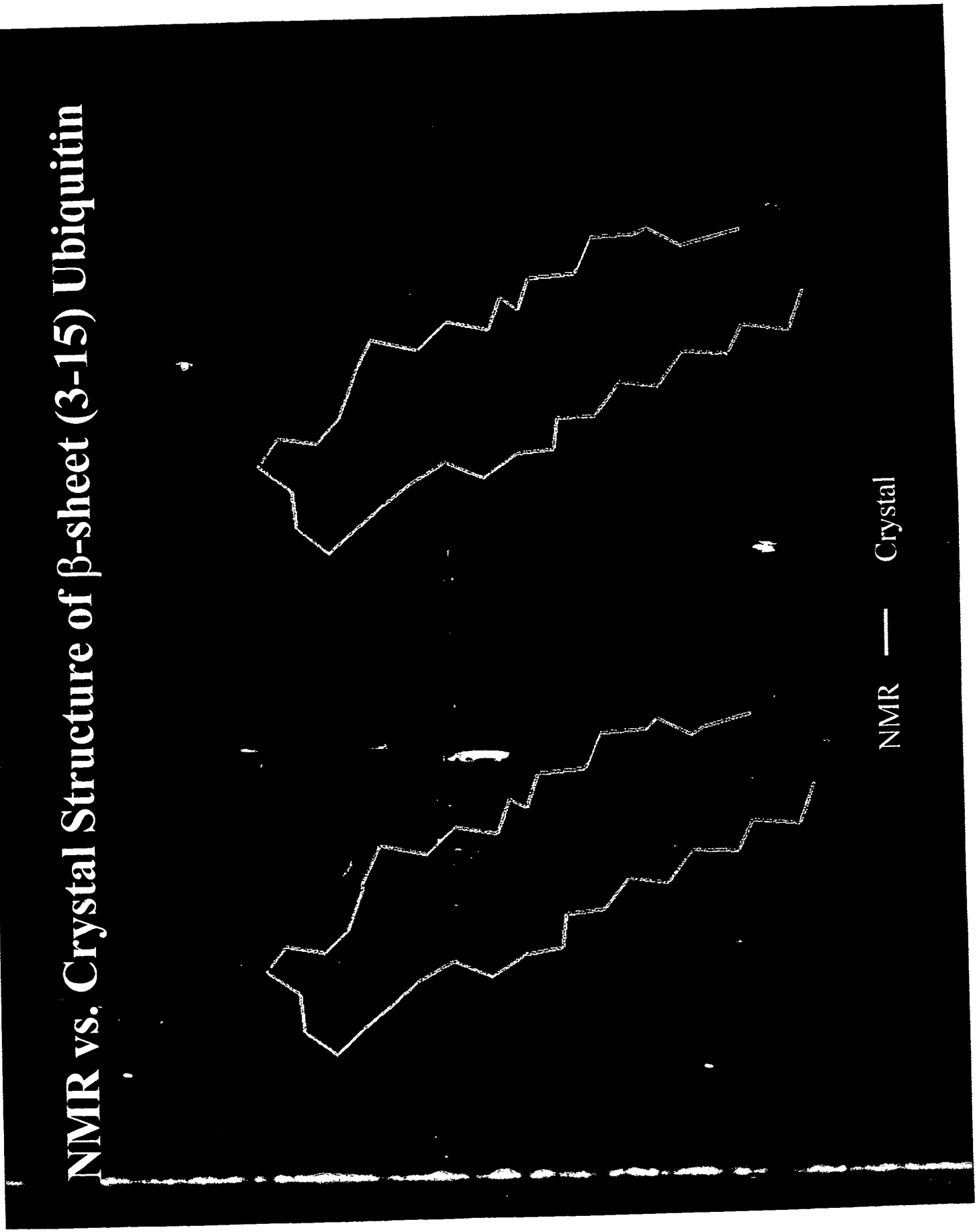
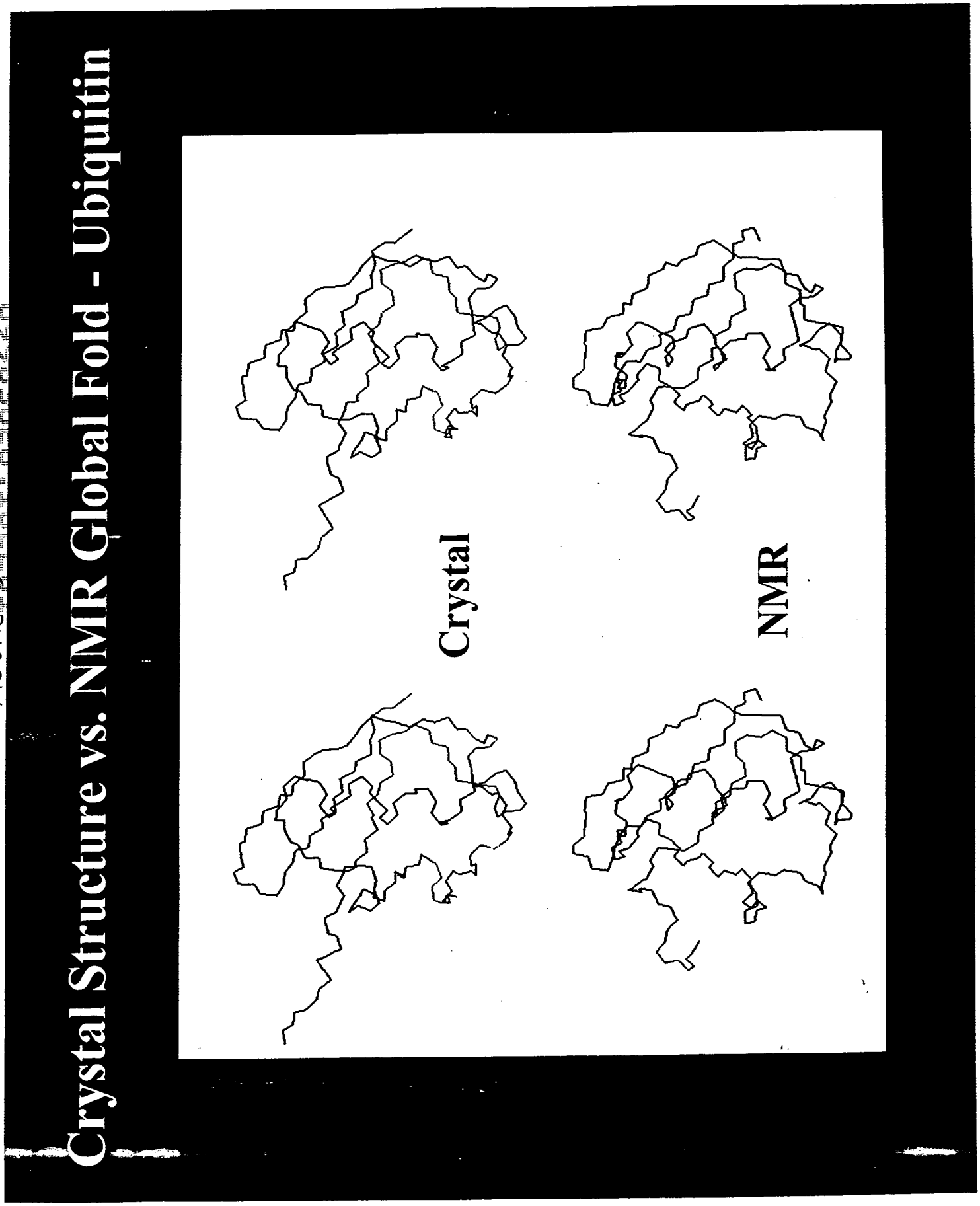

NMR vs. Crystal Structure of α-helix (24-34) Ubiquitin
NMR
Crystal

FIGURE 12


NMR vs. Crystal Structure of β-sheet (3-15) Ubiquitin
NMR — Crystal

A

FIGURE 13


Crystal Structure vs. NMR Global Fold - Ubiquitin
Crystal
NMR